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Investigation of the Effect of DamKohler and Stanton Non-Dimensional Numbers on the Stability of Continuous Stirred Tank Reactors

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ABSTRACT

The fully mixed continuous stirred tank reactor is an important and common type of industrial reactors. These types of reactors are mainly used to produce high volume products such as petrochemicals, detergents, sanitary products and products that are in demand in the market. Knowing the dynamic behavior of chemical reactors is of great importance in setting up, designing, controlling and stopping reactors. In this paper, the effect of Damkohler and Stanton dimensionless numbers on the stability of a continuous stirred tank reactor, in which a first-order exothermic reaction takes place, is atuddied. First, a mathematical model of the system's dynamic behavior was presented. Then, by simultaneously solving the equations of mass and energy around the fixed point in the MATLAB software, the effect of the mentioned numbers was investigated. The results show that the continuous stirred tank reactor shows different behaviors in different ranges of Damkohler and Stanton dimensionless numbers. This reactor behaves unstable in small and large ranges of Damkohler and Stanton numbers due to the presence of mixed or positive and negative eigenvalues. The best range for Damkohler and Stanton numbers includes numbers close to 1 because in this range the reactor shows a stable behavior due to having two negative eigenvalues. In this range, in addition to the stability, the conversion percentage is also 100 %. In this study, the ratios of Stanton to DamKohler when St / Da > 1 and St / Da = 1 were investigated. If St / Da = 1, the system is in a steady state, but in St / Da > 1, the system moves away from the steady state.

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1. Introduction

Continuous stirred tank reactors (CSTR) are among the main and most important industrial reactors. Due to the presence of a stirrer and fully mixing materials, there is no concentration gradient in this reactor, so it is

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categorized in lumped systems and the governing balance equations are in the form of ordinary differential ones [1]. The first step in studying either physical or chemical systems is to model the system into mathematical equations [2]. When the equations of CSTRs are developed in a non-dimensional form, the two dimensionless numbers of DamKohler and Stanton are obtained. DamKohler number indicates the rate of the chemical reaction to the rate of transport phenomenon in chemical systems [3], and Stanton number represents the ratio of the heat transfer flux to the heat capacity of the fluid [4]. In recent years, various nonlinear control methods have been used to evaluate the stability of agitator reactors. Bahmani and Rahmani provided a feedback control for the nonlinear system and tested its performance on two CSTR reactor systems and a quad tank. They has concluded that this method works better than some of the existing control methods for nonlinear systems [5]. The nonlinear CSTR reactor can be modeled as a linear system with time-varying parameters. Controllers, such as proportional-derivative-integral controllers, which are developed for linear systems can be applied in the CSTR reactor with time-varying coefficients [6]. A proportional-derivative-integral controller was set up to control the CSTR reactor, and using the absolute error value integral, the performance of the control system was evaluated, through which an integral error value of 0.18 was obtained [7]. In another work, a predictive control model was designed and a reactor sample was used to evaluate the effectiveness of the proposed method. Then the results of the design were compared with those of a predictive control nominal design. A superior performance of the proposed design was reported [8]. In order to optimize the CSTR reactor, a controller was designed and compared with a PI controller by Holaza et al. The construction of the pre-control was reported 25 % faster than that of the PI control [9]. They used a predictive controller to optimize the actual time and tested a model that was similar to a CSTR reactor. The proposed algorithm can improve the economic performance [10]. A predictive controller for an ODE-PDE system was discussed by Khatibi et al. The proposed controller can control the input limit and stabilize the system [11]. In another recent study, a predictive control algorithm based on a continuous discrete stochastic reduced order model was investigated and results showed that that control algorithm was able to track the temperature regulation point of an exothermic reaction in a CSTR reactor [12]. Pipino et al. designed a predictive control formula and then applied the proposed design to a CSTR reactor system [13]. Xin et al. tested an adaptive fuzzy controller on a CSTR reactor. The proposed controller can provide the internal stabilization of the closed-loop system and track the reference signals [14]. Wang et al. provided a deep learning prediction model for modeling and controlling the CSTR reactor. Learning-based predictive control showed better performance in modeling, tracking and being anti-turbulence than other advanced methods [15]. Also, various methods for tuning the controller such as genetic optimization algorithm and particle swarm [16], artificial neural network [17, 18] and optimal control [19] in controlling the reactor temperature have been studied. In previous research works, a suitable controller has been designed to control the temperature of the agitator reactor. The effect of DamKohler dimensionless numbers on the conversion

percentage [3] and reactor properties analysis by Stanton number [4] have also been investigated. Knowing the dynamic behavior of chemical reactors is of great importance in designing, controlling, commissioning and stopping them. Therefore, in this study, due to the importance of determining the dimensionless numbers of Stanton and DamKohler for the design of agitator reactors, the effects of these two dimensionless numbers on the system stability and the conversion percentage are investigated simultaneously. Finally, the best numerical values were determined for the two dimensionless numbers, DamKohler and Stanton, for the stability of a CSTR reactor system.

2. Methodology

2.1. Nonlinear systems

One of the methods for obtaining the temporal-spatial variation of variables and determining their profiles, is to develop a mathematical model of the reaction according to the type of the reaction, the type of the reactor and specific application conditions. In these cases, due to the nonlinearity and complexity of the equations, the obtained equations are seldom solvable analytically, and are generally examined in the state space and in the phase plane [20]. Sometimes in the examination of a reactor, special states are appeared. For example, a reactor may have so many sensitivities to a parameter, so either the reactor behavior may change significantly with slight changes in the parameter, or multiple states of uniformity, of which some are stable and others unstable, may occur in the reactor [21]. The phenomenon of split or branching, which causes new uniform states in different directions, due to its high speed, sometimes causes turbulence in the reactor, which makes the behavior of the reactor unpredictable [22-24].

2.2. Reactor modeling

The CSTR reactor is one of the most important and common reactors being used in the industry. Numerous mathematical theories and analytical methods have been developed for this reactor, and this reactor is at the core of studies on the multiplicity and properties of the uniform state. The system assumptions include the complete mixing, continuous and unstable reactor, physical properties of the fixed fluid, incompressible fluid, reactor volume and constant feed flow. Also, to control the temperature of the reactor, a shell, in which a fluid with a constant temperature flows, is used around the reactor [25]. Due to the variety and scope of the researches conducted on this reactor, reaction A $\longrightarrow$ B is investigated. Reaction A $\longrightarrow$ B is performed in the first instance and exothermically in a CSTR reactor.

The equations of mass and energy of the system are given in equations (1) and (2), respectively, as follows:

$$\frac{\partial c_A}{\partial t} = \frac{F}{V}\left(C_{A_0} - C_A\right) - r \tag{1}$$

$$\frac{\partial T}{\partial t} = \frac{F}{V}(T_0 - T) + \frac{(-\Delta H)}{\rho C_p} r - \frac{UA}{V\rho C_p}(T - T_C) \tag{2}$$

$$r = K C_A \tag{3}$$

where, F is the volumetric flow rate (m^3/min), V is the reactor volume (m^3), C_{A0} and C_A (Kmol/m^3) are the input and output concentrations of the component respectively,

r is the reaction rate, K is the reaction rate constant (min^{-1}), T_0 and T(K) represent the temperatures of the reactor feed and product, ΔH is the reaction heat (cal/Kmol), ρ is the fluid density (Kg/m^3), C_p is the specific heat capacity (cal/K.Kg), U is the heat transfer coefficient ($\frac{W}{m^2.K}$), A is the heat transfer surface (m^2) and T_c is the cooling fluid temperature (K) [17, 24, 2].

The dimensionless groups of the system are as follows [8, 10, 2]:

$$\gamma = \frac{E}{RT_0} \quad (4)$$

$$\theta = \frac{T}{T_0} \quad (5)$$

$$Da = K_0 \exp(-\gamma)\frac{V}{F} \quad (6)$$

$$x_A = \frac{C_{A_0} - C_A}{C_{A_0}} \quad (7)$$

$$\theta_0 = \frac{T_0}{T_0} = 1 \quad (8)$$

$$B = \frac{(-\Delta H)\, C_{A_0}}{\rho C_p T_0} \quad (9)$$

$$\tau = \frac{F}{V} \quad (10)$$

$$\theta_C = \frac{T_C}{T_0} \quad (11)$$

$$St = \frac{UA}{\rho C_p F} \quad (12)$$

The equilibrium and dynamic equations are as follows:

$$\frac{\partial x_A}{\partial t} = -x_A + Da(1 - x_A)\exp\left(\frac{\gamma\,(\theta - 1)}{\theta}\right) \quad (13)$$

$$\frac{\partial \theta}{\partial t} = (1 - \theta) + B\,Da(1 - x_A)\exp\left(\frac{\gamma\,(\theta - 1)}{\theta}\right) - St\,(\theta - \theta_c) \quad (14)$$

where, x_A is the conversion, γ is the dimensionless activation energy, B is the adiabatic temperature increment, θ is the dimensionless temperature, Da is the dimensionless DamKohler number, St is the dimensionless Stanton number, E is the activation energy, R is the global gas constant, K_0 is the impact coefficient.

It should be noted that equation (13) is due to the mass balance for component A, and equation (14) is due to the energy balance of the reactor system [25, 2].

$\theta_c = 1$, B = 8, and γ = 20 were considered as the initial values of parameters in the problem.

2.3. DamKohler and Stanton dimensionless numbers

Dimentionless Damkohler number indicates the ratio of the reaction rate to the rate of mass transfer, which the conversion perecentage at the reactor output is a function of it. DamKohler is involved in the reaction rate equation. Reactors with DamKohler numbers of less than 0.1 have low conversion rates. Therefore, increasing DamKohler number leads to increasing the conversion percentage. Therefore, DamKohler is a basic parameter for the reactor design [3]. Increasing Stanton number causes the temperature to rise at a specific time, which is called thermal runaway, a phenomenon that causes the reactor temperature to rise and sometimes cause the reactor to explode [27].

3. Results and discussion

In this study, a continuous stirred tank reactor in which a first-order reaction occurs is

modeled in the MATLAB software and diagrams of temperature and conversion versus time are obtained. First, the equilibrium points for temperature and conversion were obtained having used the equations of the mass and energy of the reactor in the steady state, and special values were calculated at equilibrium points. The steady state occurs when the eigenvalues are both real and negative numbers. Although when two numbers are real but one is positive and the other is negative, the saddle condition occurs. In this case, the parameters become infinitely asymptotic at a certain time, which causes the system instability. When the eigenvalues are complex numbers, if the real parts of these numbers are negative, the system is steady and has a limit cycle, and if the eigenvalues are complex numbers with positive real parts, the unstable state occurs. Table 1 shows the values of DamKohler and Stanton in eight cases.

Table 1

DamKohler and Stanton values in eight cases.

Case No.	1	2	3	4	5	6	7	8
DamKohler number	0.01	1	0.01	0.01	0.1	0.1	1	1
Stanton number	1	1	10	100	10	100	10	100

Figure 1 shows the reactor conversion and the dimensionless temperature versus time for case 1 (DamKohler = 0.01 and Stanton = 1). In this case, the reactor temperature is stabilized with a time delay. Also, because the DamKohler number has a low value, the conversion rate takes 10 s to reach the desired amount.

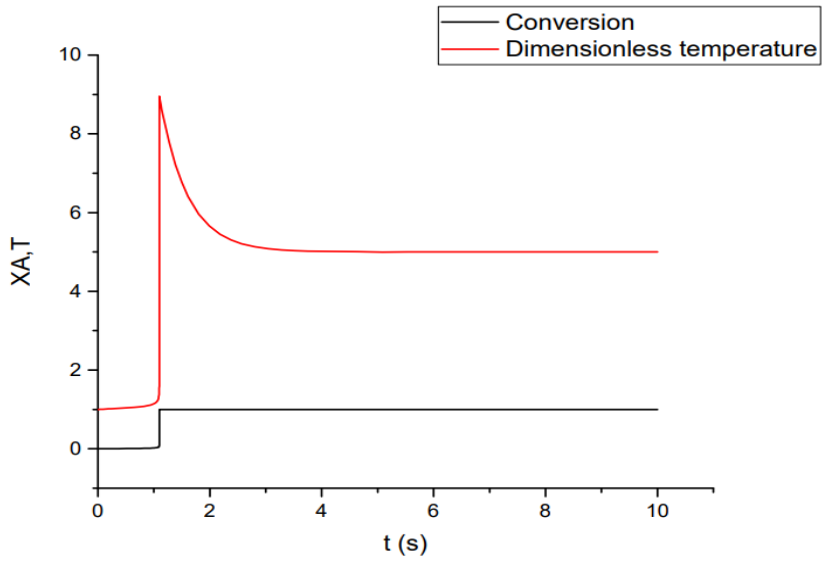

Figure 1. Conversion and dimensionless temperature versus time for the condition of case 1: DamKohler = 0.01 and Stanton = 1.

The conversion and dimensionless temperature versus time, for the condition of case 2, (DamKohler = 1 and Stanton = 1) are illustrated in Figure 2. In this case, compared to case 1, the reactor achieves the temperature stability in less time, also the second case is

superior to the first one because in this case DamKohler number is greater which causes the reaction to reach the desired conversion percentage faster.

Figure 3 shows the mentioned diagram for case 3 (DamKohler = 0.01 and Stanton = 10). This system is stable and the temperature changes are not large. But in this case the conversion rate is low.

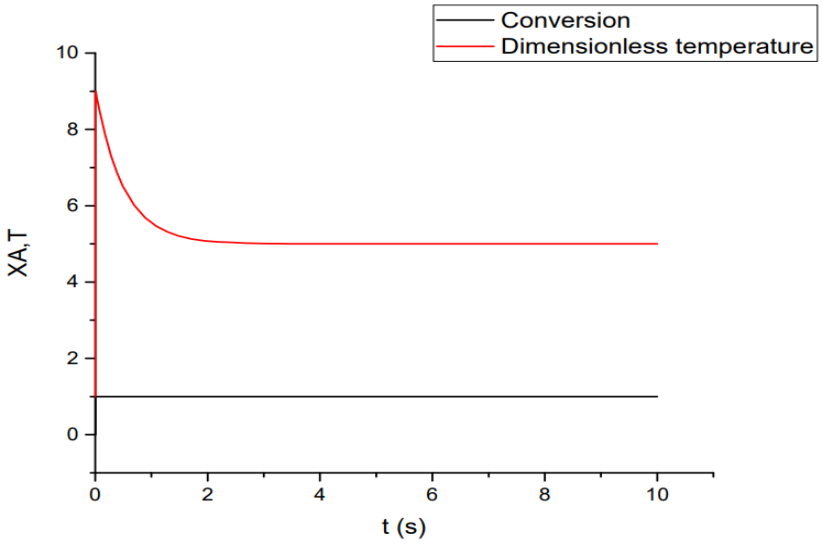

Figure 2. Conversion and dimensionless temperature versus time for the condition of case 2: DamKohler = 1 and Stanton = 1.

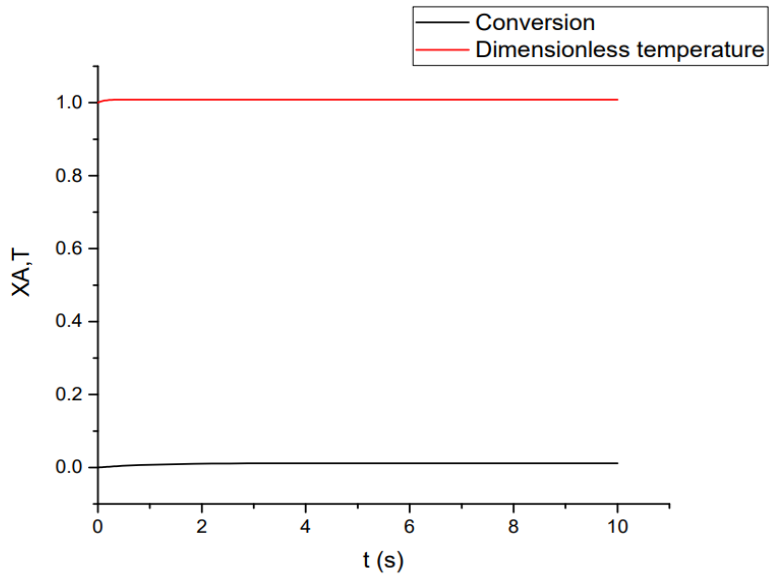

Figure 3. Conversion and dimensionless temperature versus time for the condition of case 3: DamKohler = 0.01 and Stanton = 10.

The results of case 4, in which DamKohler = 0.01 and Stanton = 100 are shown in Figure 4. The system is stable in this state. The dimensionless temperature value is 1, or in other words, the rise in temperature is not large. But the conversion in this case is the same as in case 3.

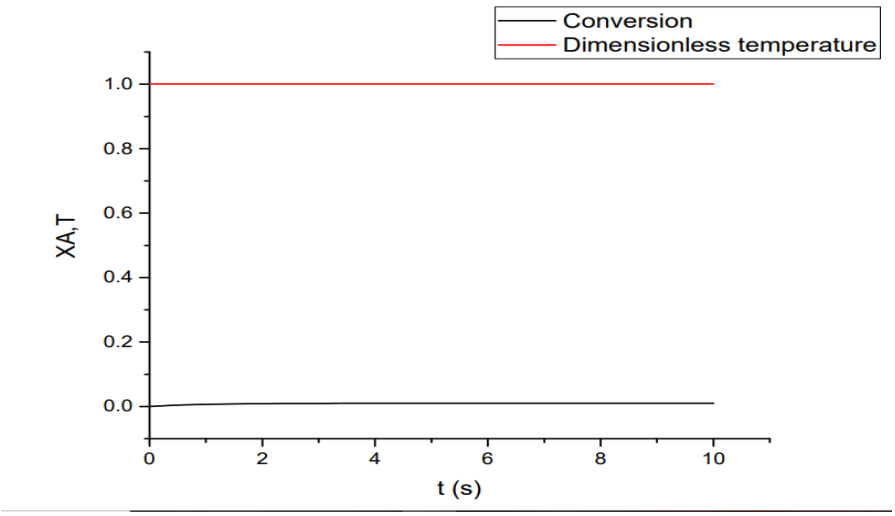

Figure 4. Conversion and dimensionless temperature versus time for the condition of case 4: DamKohler = 0.01 and Stanton = 100.

Figure 5 presents the result of case 5 (DamKohler = 0.1 and Stanton = 10). In this case, at first, the reactor temperature is stable around the dimensionless temperature of 2, but after a while (about 9 s) the system becomes unstable, which can cause problems and danger. Fluctuations in the system cause damages to the system, so it is not suitable in terms of stability. The conversion percentage in this case is close to 1.

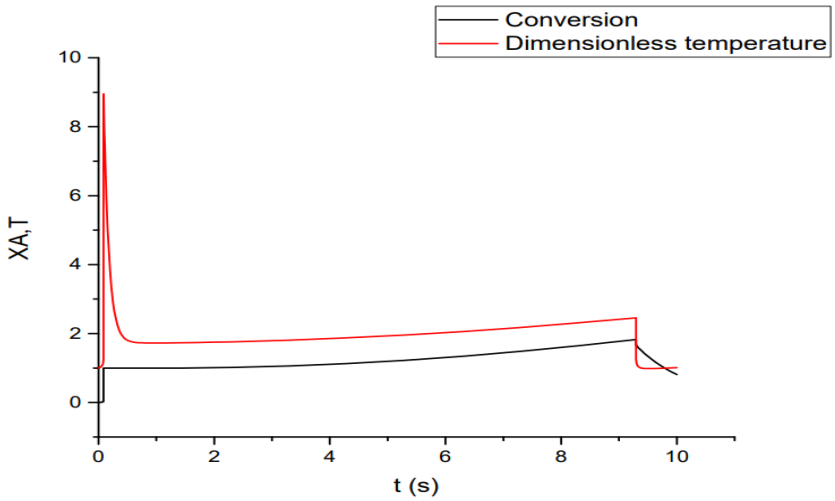

Figure 5. Conversion and dimensionless temperature versus time for the condition of case 5: DamKohler = 0.1 and Stanton = 10.

Figure 6 shows the diagrams of the conversion and dimensionless temperature for mode 6 (DamKohler = 0.1 and Stanton = 100). The system is stable in this state as shown in Figure 6. The conversion is low in this case but higher than the conversion rates in cases three and four.

Figure 7 shows the results of case 7 (DamKohler = 1 and Stanton = 10). In this case, the system is unstable, but after 8 s, it reaches a steady state. In this system, 10 s is needed for the system to reach a stable state. The amount of dimensionless temperature increases sharply at the beginning of the reactor starting up, which can cause the reactor to explode, so this is inappropriate.

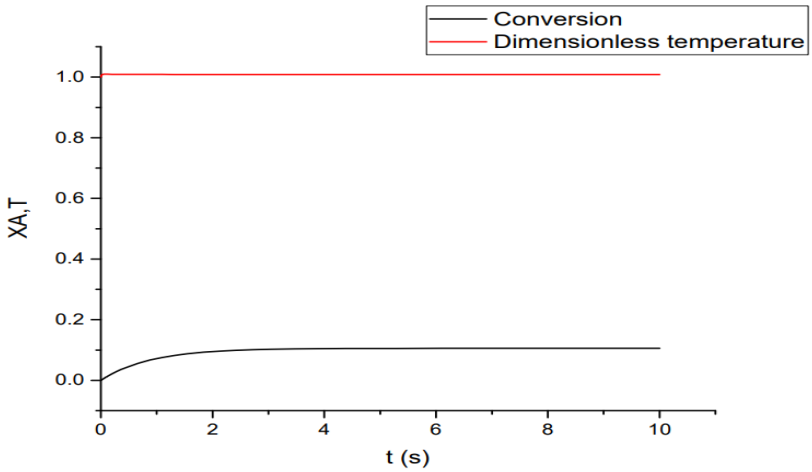

Figure 6. Conversion and dimensionless temperature versus time for the condition of case 6: DamKohler=0.1 and Stanton=100.

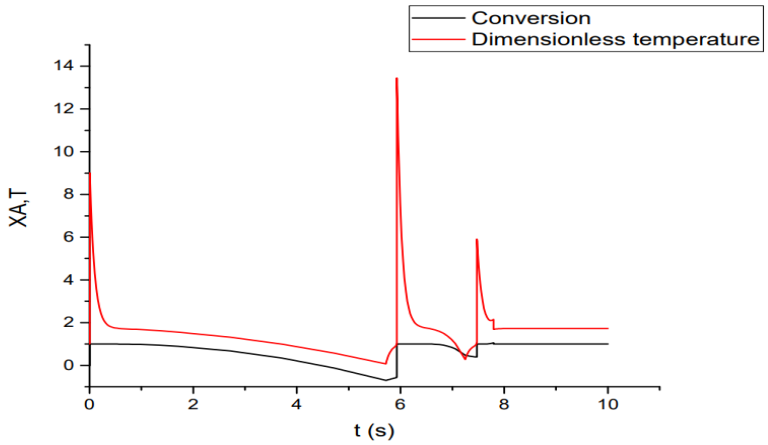

Figure 7. Conversion and dimensionless temperature versus time for the condition of case 7: DamKohler = 1 and Stanton = 10.

Finally, the results of case 8 (DamKohler = 1 and Stanton = 100), in which the system is unstable, are shown in Figure 8.

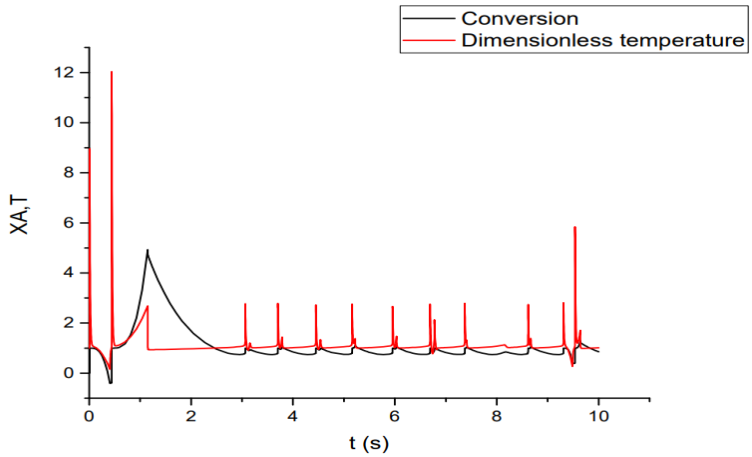

Figure 8. Conversion and dimensionless temperature versus time for the condition of case 8: DamKohler = 1 and Stanton = 100.

According to the mentioned results, when the numerical value of DamKohler was selected as 0.01, the conversion percentage at the reactor output decreased. This result is in good agreement with that of a recent study [3] which shows that reactors with DamKohler numbers less than 0.1 have low conversion rates. Also, a high value of Stanton number would cause the system instability. Zaldivar et al. have also reported that increasing Stanton number is the reason for the increase in temperature and the explosion of the reactor, which is one of the reasons for instability [27]. In this study, we have also examined the ratio of the two numbers of Stanton and DamKohler in two cases. If $\frac{\mathrm{St}}{\mathrm{Da}} \approx 1$, the system is thermally stable and high conversion can be achieved. When $\frac{\mathrm{St}}{\mathrm{Da}} \gg 1$, simillar to the other report [27], the system is thermally stable, but the convesrion depends on Da number, so that in $\mathrm{Da} \geq 0.1$ the conversion is high and in $\mathrm{Da} < 0.01$ it is low. Finally, in the range of $1 < \frac{\mathrm{St}}{\mathrm{Da}} < 100$, the system is unstable.

5. Conclusions

This work is a stability analysis of a the CSTR reactor system for an initial exothermic reaction. To evaluate the stability of the CSTR reactor, first the mass and energy modeling based on the two dimensionless numbers of DamKohler and Stanton was performed by the MATLAB software. Then the effect of different values of Stanton and DamKohler on the system stability and the percentage of the reactor conversion was investigated. As the value of Stanton number increases, a thermal runaway occurs, which causes the system to become unstable, but an increase in DamKohler number increases the conversion percentage. So, three cases can be considered for these numbers. The first case is that Stanton number is close to 10 and DamKohler number is close to 0.01. In the second case, Stanton number should be close to 10 and DamKohler number should be close to 0.1, and the third case should be with Stanton number close to 100 and DamKohler number close to 0.1, which, according to these results the best range for DamKohler number and Stanton is being close to 1 because in this case, in addition to system stability, the conversion rate is also high. In this study, the ratios of Stanton to DamKohler when St / Da > 1 and St / Da = 1 have been investigated. If St / Da = 1, the system is in the steady state, but when St / Da > 1, the system moves away from the steady state.

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